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Experimental application of nonlinear model predictive control: temperature control of an industrial semi-batch pilot-plant reactor

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Abstract

This paper describes the application of nonlinear model predictive control (NMPC) to the temperature control of a semi-batch chemical reactor equipped with a multi-fluid heating/cooling system. The strategy of the nonlinear control system is based on a constrained optimisation problem, which is solved repeatedly on-line by a step-wise integration of a nonlinear dynamic model and optimisation strategy. A supervisory control routine has been developed, based on the same nonlinear dynamic model, to handle automatically the fluid changeovers. Both NMPC and supervisory control have been implemented on a PC and applied to a 16 l batch reactor pilot plant. Experiments illustrate the feasibility of such a procedure involving predictive control and supervisory control.

Keywords: Industrial semi-batch reactor; Nonlinear predictive control; Supervisory control; Temperature control

1. Introduction

Batch or fed-batch reactors are frequently used to manufacture high-added-value products in the pharmaceutical and fine chemical industry. Their flexibility and operation similarity to the bench-scale laboratory reactor make their use attractive. However, in order to improve the quality of the products and to ensure uniform production from one batch to another, it is necessary to improve the automation of these reactors. Several industrial heating/cooling configurations are used for their thermal control. This study focuses on the alternative-fluid (multi-fluid) system mainly used in industry (90% of the cases) as pointed out in [1,2]. The alternative-fluid system consists in delivering a hot or cold fluid, each one available at a constant temperature, to the jacket of the reactor. The reactor temperature is controlled by manipulating the flowrate of the utility fluid. A typical operation of a batch or semi-batch reactor, consists of the tracking of an a priori defined temperature profile (in the case of an exothermic reaction, three distinct steps are involved: preheating, reaction and cooling). In industrial practice, the changeovers from one utility fluid to another always involve an air purge of the jacket (especially in the case of a change from glycol water to mains-water to avoid glycol over-consumption). Consequently, this causes an abrupt change in the dynamics marked not only by a change in the characteristics of the utility fluid but also by a discontinuity due to the intermediate air purge and the refilling of the jacket. Coupled with the nonlinear reactor model structure, uncertainty in the model parameters and unknown disturbances, the complexity of the batch reactor temperature control makes this a challenging problem. To handle correctly the utility fluids to be injected into the jacket as well as the intermediate air purge and the refilling during the changeover of the fluid, a supervisory routine has been proposed by Ettedgui [3] based on online determination of future temperature trajectories obtained for minimum and maximum thermal capacities of each fluid.

Nonlinear control systems, including strategies using explicitly a dynamic nonlinear model of the process for the development and implementation of a control system,

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have been the subject of an increasing interest. Amongst them one can cite two principal types, one based on Differential geometry [4–6] and the other being nonlinear model predictive control (NMPC) [7,8]. The former type, with a strong theoretical basis, has produced efficient results corroborated by application to various processes through simulation studies mainly. This technique suffers of some cumbersome limitations in experimental implementation due to its incapability to handle properly amplitude and velocity constraints on the manipulated variables. The latter type although demanding a generally greater computing effort, offers the advantage of greater flexibility, easily integrating system delays and various constraints (which might not be avoided in industrial processes due to safety requirements, quality control or equipment design limitations). Similarly, very few experimental applications can be noted. A comprehensive review of this topic as well as other nonlinear control strategies for chemical processes has been provided by Bequette [9].

In contrast with adaptive control strategies which are often based on a "black box" model (i.e. input–output model) not related to any physical/chemical phenomena involved in the process, MPC allows the explicit integration of phenomenological process models in the control system [10]. In the case of a nonlinear dynamic model, there is no more an analytical solution of the problem. The predictive control strategy is thus based on a repeated optimisation of a performance criterion subject to various constraints over a finite future time horizon. It involves thus a real-time selection of a set of future manipulated variable moves so as to minimise an objective function often based on the square errors between the predicted model output and a desired output trajectory over a prediction horizon. Different solutions have been proposed in the literature.

Biegler [11] first used the collocation technique to transform the DAE model into algebraic equations, which enter as constraints in the NLP problem. The resulting constrained control problem is then solved via nonlinear programming (NLP). The main problem of this solution is that the number of decision variables quickly increases with the number of states as these ones become decision variables by the collocation technique.

Another solution proposed by Ricker and Lee [12] is based on the use of a linear model of the plant (obtained by linearising the nonlinear model at each sampling period) in the projection/prediction step. The NLP problem is then transformed into a QP problem. As mentioned by the authors, this technique will give good results if the non-linearities are not too strong. In our case, the process concerned is a batch one, which does not reach steady state. Moreover, it exhibits strong and abrupt changes in dynamics due to specific operation steps (air purge of the jacket).

In this work, the DAE system is solved over the prediction horizon at each iterative step of the NLP procedure optimisation step. A classical DAE solver (Gear method) has been used. It is similar to the approach used by [13] who applied it in a simulation study to the control of a reactive distillation column and used by [8] for the control of a laboratory scale fixed-bed water–gas shift reactor.

The dynamic model of the batch reactor constituting the DAE system was obtained from mass and energy balances. To avoid partial derivative equations describing the flow rate inside the jacket, this latter has been lumped into a succession of perfectly mixed tanks [14,15]. The overall dynamic model is composed of $4+2*(N_t\text{-}2)$ differential equations, where N_t is the number of tanks describing the jacket hydrodynamics. The resolution of the set of equations only needs the reactor geometrical specifications and the initial temperature conditions (the reactor temperature, the inlet and outlet jacket temperatures are measured variables and the reactor wall, the jacket wall temperatures are computed variables). There are almost 40 geometrical parameters needed to describe properly the geometry of the batch reactor among them: inlet diameter of the jacket, thickness of the jacket wall, of the reactor wall, dimension of the stirring device, ... which are used in the various correlations enabling the on-line computation of the heat transfer coefficients. These parameters are generally given by the reactor provider (the authors can provide details of models and the reactor parameters to any interested reader who will make an e-mail request). With these specifications, the dynamic simulation model remains very generic and can be used to simulate any type of jacketed reactor. It has been experimentally validated for different types of reactors (from 1 to 1000 l, stainless-steel or glass-lined) [14].

In our case the system is composed of 14 differential equations (7 issued from the jacket discretisation). At every changeover of utility fluid, the model is changing at least by means of the value of heat transfer coefficients which are computed on-line. Furthermore, during a changeover, two differential equations are added to model the presence of two fluids inside the jacket and a moving interface of the liquid inside the jacket during the filling or the air purge.

As mentioned in [2], very few experimental studies on application of NMPC are reported in literature. In [8], the authors applied the NMPC to a continuous process. In our case, the process is a batch one and consequently there is no steady-state. Moreover, as it has been previously mentioned, at every changeover of utility fluid, the model is changing in its parameters (heat transfer coefficients) but also in its structure (two supplementary states are introduced).

This dynamic model is also used to perform a supervisory control to handle correctly the fluid changeovers based on the predicted temperatures. The complex dynamic model is, therefore, used not only for control

purposes by means of the NMPC but also in the supervisory control aspect. It becomes the heart of the overall supervisory control and regulation procedure. The main contribution of this paper is to show experimental results of the application of such a technique on an industrial batch process: a glass-lined 16 l reactor.

2. The pilot plant

This pilot plant consists of a stirred glass-lined batch reactor fitted out with a multi-fluid heating/cooling system (Fig. 1). A schematic diagram of the heating-cooling system is depicted in Fig. 2.

Air is used to empty the jacket when changing the utility fluid. Four utility fluids are available at a given temperature: steam, cold water, hot water and a mixture of monopropylene glycol and water (50/50 weight). The hot water stream is obtained by mixing steam and cold water to produce hot water at 70 °C. In practice, hot water is produced by fixing the cold water flowrate and computing, via an energy balance on the mixer, the necessary steam flowrate to produce water at 70 °C. The pilot reactor is fitted out with sensors of temperature, pressure and flowrate for every fluid. Seven temperature sensors (Pt100) are used to measure the following temperatures: jacket inlet temperature, jacket outlet temperature, mixer outlet temperature, cold water inlet temperature, steam temperature, reactor temperature, jacket wall temperature. Four sensors are used to measure the following values: glycol/water, cold water, hot water and steam

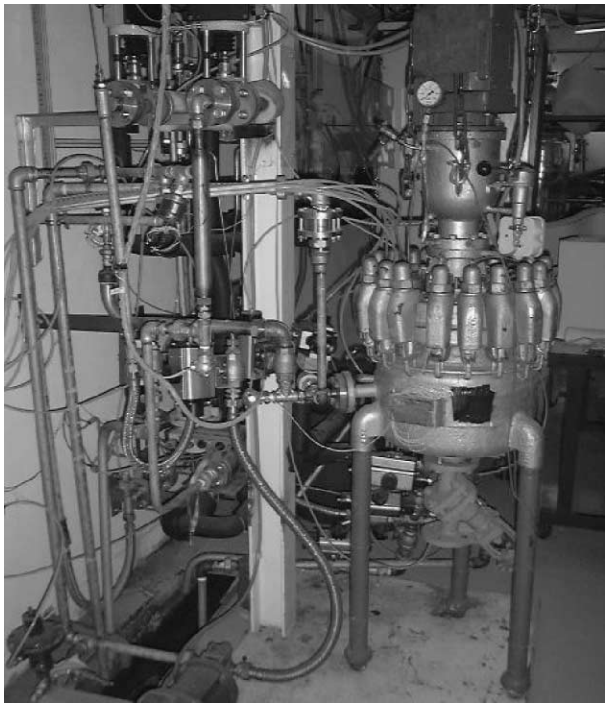

Fig. 1. The batch reactor pilot-plant.

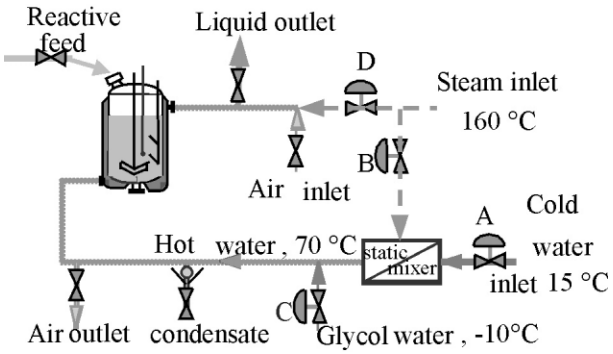

Fig. 2. The multi-fluid system.

flowrates. The actuators on the pilot plant include two types of valves: on-off valves and proportional valves. Four proportional valves are available which allow controlling the flowrates of thermal fluids available on the pilot plant as follows:

- cold water flowrate (A)
- steam flowrate (D)
- steam to be mixed with cold water flowrate (B)
- glycol/water flowrate (C).

Valves A and B are moved simultaneously to change the hot water flow whilst the valve positions are determined to satisfy the mass and energy balances for the desired flowrate at 70 °C.

3. Experimental results

To demonstrate the good performance of the control methodology and the supervisory procedure, different experiments have been carried out on the pilot plant reactor previously described. The reactor has been charged with 10 l of water.

In this study, experiments involve chemical reactions which have been simulated using heat source for exothermic reactions. For safety and experimental cost saving, the pilot plant reactor has been fitted with heating resistances. This device allows to "simulate" the generation of heat during an exothermic chemical reaction as described in [16]. The heat generation rate is computed on-line according to the kinetic model of the chemical reaction concerned. This value is then applied to the process by means of heating resistance. In our case, the chosen reaction is the reaction between thiosulfate and peroxide which is known to be highly exothermic:

$$Na_2S_2O_3 + 2H_2O_2 \rightarrow 1/2Na_2S_3O_6 + 1/2Na_2SO_4 + 2H_2O \quad (1)$$

The advantage of the simulation of the chemical reaction thermal effect is to prevent run-away problems,

which can occur experimentally, particularly for such a reaction.

The expression for the reaction rate is:

$$r = kC_AC_B = k_0\exp(-E/RT)C_AC_B \tag{2}$$

where $A = Na_2S_2O_3$, $B = H_2O_2$, $k_0 = 2\times10^{10}$ m^3 kmol^{-1} s^{-1} and $E = 1.63\times10^4$ kcal kmol^{-1}.

The heat generation profile (for the experiment in Fig. 4) applied by means of the heating resistances is given on Fig. 3. This profile corresponds to the reaction of 3.4 kg of $Na_2S_2O_3$ in 10 l initially present in the reactor with a H_2O_2 feeding rate of 1.6×10^{-2} kg s^{-1}.

Different simulation and experimental studies have yielded information on the way to choose the controller design parameters [17]. The optimisation problem can be summarised by:

Objective function

$$\mathrm{Min}J(k)\sum_{i=HP1}^{P}\left[\, y_{\mathrm{ref}}(k+i) - y_{\mathrm{pred}}(k+i)\,\right]^2 \qquad u(k+1),\ldots,u(k+N) \tag{3}$$

subject to constraints:

Dynamic model equations

$$\frac{\mathrm{d}x(t)}{\mathrm{d}t} = f(x(t), u(t), l(t), w(t), p) \tag{4}$$

Algebraic output equation

$$y_{\mathrm{m}}(t) = h(x(t)) \tag{5}$$

Upper and lower bounds on manipulated variables

$$u_{\min} \leqslant u(k+i) \leqslant u_{\max} \quad i = 1, .., N \tag{6}$$

Upper and lower velocity bounds on manipulated variables

$$u(k+i-1) - \Delta u_{\max} \leqslant u(k+i) \leqslant u(k+i-1) + \Delta u_{\max} \quad i = 1,\ldots \mathrm{N} \tag{7}$$

Initial conditions

$$x(k) = x_k \tag{8}$$

where: k is the sampling time, *HP1*, P are parameters that allow the definition of the prediction window in which the process output is wanted to track the reference trajectory y_{ref}, u is the manipulated variable, x the state space vector, y_{m} the process model output, y_{pred} the predicted process output, l the measured load disturbance vector, w the unmeasured load disturbance vector, p the model parameter vector. At each sampling time k the model state vector, $x(k)$, has to be initialised. x_k is either the current measured state vector or the current process model output vector in the case of output disturbance estimation (in order to ensure a zero offset at steady state).

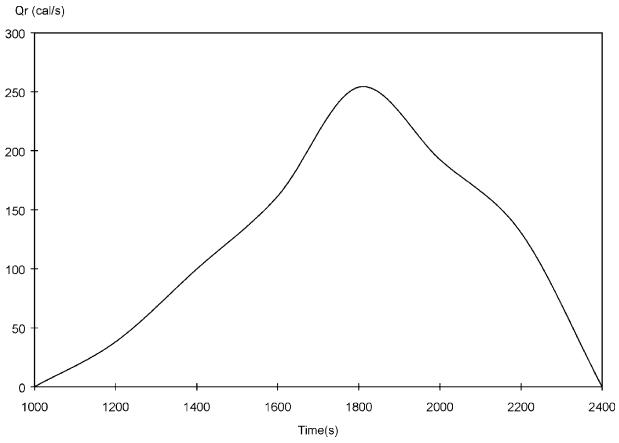

Fig. 3. The heat generation rate profile for the first experiment.

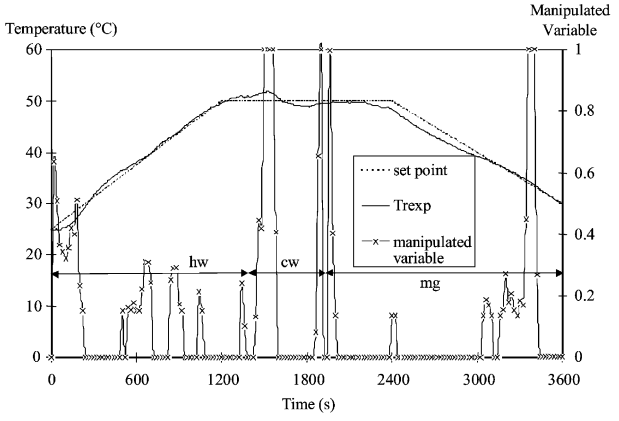

Fig. 4. NMPC temperature control with a partially simulated chemical reaction (reaction temperature at 50 °C).

Feedback is incorporated via an output disturbance estimation. In this case, the model/plant mismatch is estimated at the kth sampling time by:

$$d(k) = y_{\mathrm{mes}}(k) - y_{\mathrm{m}}(k) \tag{9}$$

where $y_{\mathrm{mes}}(k)$ is the current measured process output. Different possibilities can be used for the correction of the process model. The simplest one considers that the model/plant mismatch is constant over the prediction horizon in this case:

$$y_{\mathrm{pred}}(k+i) = y_{\mathrm{m}}(k+i) + d(k+i) \quad i = 1,\ldots,P \tag{10}$$

Most often, velocity constraints on the manipulated variable are not explicitly expressed but are treated via additional weighted terms in the objective function to penalise the move sizes. We deliberately use a formulation of the problem with explicit constraints (called also

"hard" constraints) both on the manipulated variable magnitude and velocity. In this case, the constraints are guaranteed to be always satisfied what it is not true in the case of using penalty functions (also called "soft" constraints). In the latter case, the result will mainly depend on the value of the weighting parameters in the objective function.

The problem of temperature control of a batch reactor fitted out with a multi-fluid system can be viewed globally as a MISO problem: the process output is the reactor temperature and the inputs are the actions on the different control valves. Since only one fluid can be present in the jacket, a supervisory control procedure is needed to choose the right utility fluid and therefore to transform this MISO problem into a succession of SISO problems where the manipulated variable is the opening degree of the valve corresponding to the chosen utility fluid: valve C for glycol water, valve D for steam, valve A for cold water, valves B and A for hot water.

In this paper, the formulation presented by [12] for the representation of the manipulated variable has been adopted. The prediction horizon P, is divided into N blocks (each block containing one or more sampling periods). The manipulated variable is then held constant within each (time) block. The number of decision variables is consequently equal to the number of blocks. It has several advantages: to decrease the number of decision variables but mainly it allows to look for an optimal input profile with constant values uniformly shared on the prediction horizon (instead of searching two different values for the first two future times and considering that the manipulated variable is constant on the rest of the prediction horizon). This generally leads to smooth the control action [3].

The key controller design parameter is the prediction horizon. In simulation, the longer the prediction horizon is, the better the control performance (in term of anticipation) is. As far as an experimental application is concerned, the problem is different since there is plant model/ mismatches that may cause a deviation in the predictions which becomes bigger and bigger as the prediction horizon is increased. So, there is a compromise between a prediction horizon that is long enough to ensure a good anticipation but not too long to degrade the predictions due to a plant/model mismatch [17]. Nevertheless, experimental studies [15] have shown that there is a reasonable margin and that a good compromise is obtained by setting this value equal to once or twice the process time-constant. For the other controller synthesis parameters there exists also a large range of admissible values.

For this experiment, the following controller design parameters have been chosen:

- a sampling period of 20 s: the time constant of the process has been approximated to 180 s, dividing this time constant by 10 leads to a suitable value of the sampling period.
- a time delay of one sampling period
- a prediction horizon of 9 sampling periods (i.e. a prediction horizon equal to the time constant of the process)
- 2 control moves as decision variables uniformly shared with 4 blocks each.

The NLP problem is solved by a reduced gradient optimisation algorithm [18] which can handle linear and non linear constraints.

As previously mentioned, the choice of the appropriate fluid is done by the supervisory controller which determines on-line the future temperature trajectories obtained for minimum and maximum thermal capacities of each fluid by using the same dynamic model. For example, if the jacket is presently fed with steam and if the measured reactor temperature is inferior to the inlet steam temperature then the maximum temperature trajectory (on the prediction horizon) is determined by integration of the dynamic model with as input, the maximum steam flowrate. The minimum temperature trajectory is computed by considering the scenario of an air purge. Of course, if the future set point trajectory is not within these limit trajectories, the supervisory controller chooses the appropriate fluid, else the present fluid is kept to minimise the number of fluid changeovers.

The whole regulatory control and supervisory control procedure has been implemented on a PC 486. The 20 s sampling period was sufficient for the convergence of the optimisation problem at each step. The decision variables of the optimisation problem (the control moves) are initialised with the values obtained at the previous period, so generally the solution is not far from the former point. The main difficulty occurs when there is a changeover of utility fluid and when the model is changing (purge, filling, ...). Nevertheless, at each iteration a call to the internal clock allows to know the remaining time before the next acquisition. In the case of a non convergence within this sampling period, the developed procedure consists in choosing the solution which gives the smaller value of the objective criterion. Let us notice that during the experiments presented in the following this case did not occur.

Figs. 4 and 6 present the time evolution of the reactor temperature, the temperature set point and the manipulated variable corresponding to the heat generation rate profiles given respectively in Figs. 3 and 5. Each experiment corresponds to a different temperature set point profile with as desired temperature of the reaction step: 50 °C for the first experiment (Fig. 4) and 60 °C (Fig. 6) for the second one. In both cases the reaction is simulated between 1200 and 2400 s. The notations hw, cw, mg mean that the fluid used is

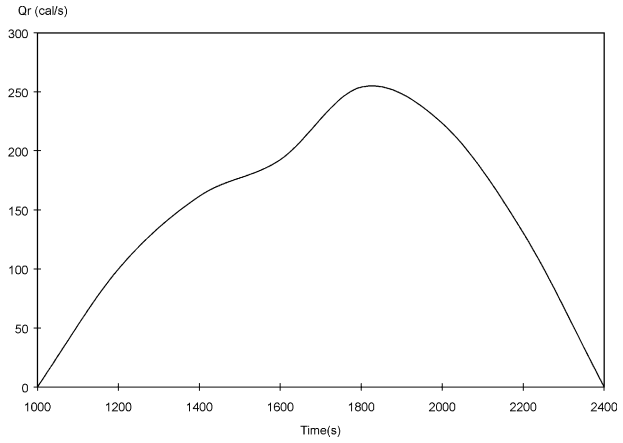

Fig. 5. The heat generation rate profile for the second experiment.

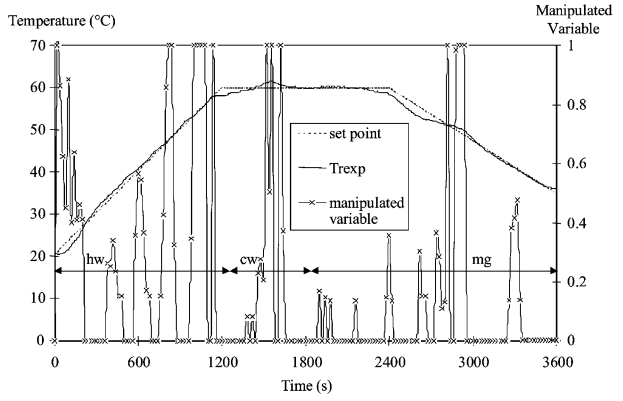

Fig. 6. NMPC temperature control with a partially simulated chemical reaction (reaction temperature at 60 °C).

respectively hot water, cold water and monopropylene glycol.

The controller design parameters are the same in both experiments. It can be noticed that, the generation rate of heat produced by the chemical reaction is considered as a disturbance (no a priori information was included in the dynamic model).

It has to be noticed that the valve B used to produce hot water exhibited a dead zone between 0 and 0.15 (for a control action corresponding to a value within this interval, the resulting opening degree is 0 or 0.15).

For both experiments, the supervisory control procedure chose hot fluid for the preheating phase. A difference of less than 1 °C can be observed during this phase. At time 1200 s, the heat generation is "simulated" via the two heating resistances. There is a small overshoot (in the case of Fig. 4) which is rapidly reduced by a corrective reaction of the controller. In both cases, the supervisory control procedure has chosen the monopropylene glycol during the reaction step due to the exothermicity exhibited by this specific reaction (with a maximum heat generation at 1800 s which corresponds to this changeover to monopropylene glycol). As this fluid was suitable to ensure the final cooling phase, the supervisory control routine kept this choice. When monopropylene glycol is used, a slightly bigger difference between the reactor temperature and its set point appears. This corresponds to the end of the "simulated" reaction. Let us recall that the heat generation rate has not been considered in the dynamic model, and this led to a plant model mismatch. The correction is done gradually by the error compensation technique [Eq. (9)]. Once this correction has been performed, the temperature follows its set point trajectory perfectly.

In order to obtain a better control performance, studies are presently devoted to incorporate an on line estimator of the heat production rate during reaction, within the NMPC dynamic model but also within the supervisory controller. More precisely an estimation of the dynamic evolution of the heat generation rate over a past finite horizon will permit the addition of feed-forward information in the predictions.

4. Conclusions

Non-linear model predictive control has successfully been applied to the thermal control of a semi-batch reactor. The strategy of NMPC coupled to model-based supervisory control, based on a complex dynamic model, was applied for the temperature control of the batch reactor (on a real industrial glass-lined pilot-plant of 16 l) equipped with a multi-fluid system. The complex dynamic model used for prediction in NMPC and in the supervisory control procedure describes the thermal behaviour of the fluid inside the jacket during special steps: air purge and filling. The main contribution of this study is the experimental application of a technique allowing simultaneously the supervisory control and the regulation by using the same complex dynamic model. Experiments involving "partially simulated" reactions have shown very good performances of the overall NMPC and supervisory controller.

As mentioned previously, an on-line estimator of the heat-released rate will be incorporated in the overall structure to feed the dynamic model with this useful information. These studies are made in collaboration with pharmaceutical industry where the kinetics of the reaction are not known and where there is a crucial lack of on-line measurement of concentrations, requiring thus the development of an on-line estimator.

Finally, structuring the control variable as a polynomial law of time (instead of N step constant values) should be investigated to minimise the optimisation computation effort during searching more complex control trajectories: the parameters of the polynomial law becoming the decision variables of the NLP problem in this case.

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